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ETHYL CORPORATION

Inter-Office

August 19, 1985

TO:

Mr. D. E. Park

ADDRESS: H

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FROM:

J. W. Parson

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SUBJECT:

Calculation of Equivalent

Concentrations of 2.3,7,8-TCDD at Sauget

Attached is a report which discusses the procedures and results of calculations of equivalent concentrations of 2,3,7,8-TCDD at Sauget based on the EPA Chlorinated Dioxin Work Group Position Document.

J. W. Parson

JWP/isd

Attachment

cc: Mr. D. C. Bach

Dr. G. L. Ter Haar Mr. S. E. McWilliams

ETHYL PETROLEUM ADDITIVES - SAUGET, ILLINOIS (CDDs)

- I. Analytical Data Chlorinated Dibenzo Dioxins (CDDs) and Chlorinated Dibenzo Furans (CDFs)
- II. Calculation of Equivalent Toxicity, as 2,3,7,8-TCDD, of a complex mixture of CDDs and CDFs using Toxic Equivalency Factors

I. Analytical Data

Soil samples taken under Administrative Order

V-W-007-84 were analyzed for were analyzed for 2,3,7,8-TCDD

and other tetra-, penta-, hexa-, hepta- and octa chlorinated

CDDs and CDFs by Envirodyne Laboratories. The results of

these tests were submitted to USEPA Region V on July 29,

1985. The data are summarized in Table I.

TABLE I

ETHYL PETROLEUM ADDITIVES - SAUGET, ILLINOIS
CHLORINATED DIBENZO DIOXINS AND CHLORINATED
DIBENZO FURANS IN SOIL

			Concentration (ppb)									
		Depth	2,3,7,8									
Sample	Location	Inches	TCDD	<u>PCDD</u>	<u>HCDD</u>	<u>HPCDD</u>	<u>OCDD</u>	TCDF	PCDF	HCDF	HPCDF	OCDF1
1	10N-180E	0-2	ND ²									
2	550N-10E	0-2	ND									
3		0-2	0.68									
4	1510N-310E	0-2 0-2	ND									
	620N-720E	0-2 0-2	0.24									
5	880N-240B	0-2 0-2	11.0									
6	970N-340B											
7	810N-360E	0-2	4.9									
_		12-18	2.3									
8	970N-560B	0-2	1.4									
9	970N-530B	0-2	9.4									
		12-18	0.31	ND	ND	ND	0.40	0.064	0.032	ND	ND	ND
10	930N-560B	0-2	2.6									
		12-18	1.6	ND	1.6	0.57	ND	0.089	0.16	0.34	0.15	ND
11	930N-230R	0-2	51.0									
		12-18	161.0	ND	ND	ND	0.71	2.6	1.6	0.074	ND	ND
		24-30	86.0									
		36-42	5.4									
		48-54	12.3									
12	880N-530E	0-2	110									
		12-18	286.0					•				
		24-30	3.0	ND	ND	ND	ND	0.86	0.49	ND	ND	ND
		36-42	0.77									
		48-54	0									
		0-6	3.9									
13	980N-305E	12-18	0				:					
14	910N-300E	0-6	0.33									
15	850N-300B	0-6	ND									
16	800N-300E	0-6	ND									
17	730N-300B	0-6	4.4							•		

TABLE I (Cont'd)

							oncent	ration	(ppb)			
		Depth	2,3,7,8									
<u>Sample</u>	Location	Inches	TCDD	PCDD	<u>HCDD</u>	HPCDD	<u>OCDD</u>	TCDF	PCDF	<u>HCDF</u>	HPCDF	<u>ocdf</u>
18	960N-370E	0–6	100.0									
10	300M-370B	12-18	70.9									
		24-30	107.0	2.1	3.5	1.4	2.5	8.1	5.9	2.0	1.0	0.11
		36-42	12.0	2.1	3.5	1.7	2.5	0.1	3.3	2.0	1.0	0.11
		48-54	0									
19	980N-360E	0-6	6.3									
20	770N-330B	0-6	5.3									
21	970N-320B	0-6	1.5									
22	480N-740E	0-6	0.64									
23	370N-740E	06	0.95									
24	910N-470E	0-6	2.4									
		12-18	3.2	0.55	0.62	0.35	0.18	0.39	0.36	0.26	0.10	ND
25	815N-505K	0-6	1.2			•						
26	910N-600E	0-6	ND									
27	1010N-540E	0-6	0.10									
28	980N-470E	0-6	5.8									
29	615N-300B	0-6	0.14									
30	820N-160R	0-6	ND									
31	1080N-205E	0-6	0.43									
32	1080N-360E	0-6	1.0									
		0-6	1.8									
33	1080N-315E	12-18	0.24									
34	1240N-300B	0-6	ND									
		0-6	1.9									
35	1280N-415E	12-18	0									
36	1540N-140E	0–6	1.3									
37	880N-390E	Sewer	13.5				:					
		Sludge					:					
38	160N-105E	0-12	0									
39	260N-30E	0-6	0									
40	115 N -10R	0-6	0								•	
41	530N-85E	0-6	0									

TABLE I (Cont'd)

. • •						C	oncent	ration	(dqq)			
<u>Sample</u>	<u>Location</u>	Depth <u>Inches</u>	2,3,7,8 TCDD	PCDD	HCDD	HPCDD	OCDD	<u>TCDF</u>	PCDF	HCDF	HPCDF	OCDF
42	360N-380B	0-6	0									
43	1015N-200E	0-6	0									
44	1000N-700E	0-6	0									
45	1200N-700E	0-6	0									
46	1030N-630E	0-6	0									
47	1100N-630E	0-6	0									
48	240N-160B	0-6	0									
49	450N-320B	0–6	0									
50	1490N-380K	0-6	0									
51	920N-620B	0-6	0				•					
52	730N-610E	0–6	0									
53	895N-370B	0-6	0									
54	850N-540B	0-6	0.98									
		12-18	0.57									
		24-30	0.08									
55	980N-430E	12-18	2.4									
		24-30	39	1.3	4.5	6.6	2.0	26.2	22.3	3.1	0.98	0.11
56	980N-480E	0-6	0									
57	930N-430B	0-6	6.2	ND	21.8	329	635	ND	3.3	28.5	70.4	29.3
		12-18	0.24									
58	1040N-385E	0-6	0									
59	1050N-300E	0-6	1.3									
		12-18	0.43									
60	730N-280B	0-6	0									
61	830N-430E	12-18	0									

TABLE I (Cont'd)

							oncent	ration	(ppb)			
Sample	Location	Depth <u>Inches</u>	2,3,7,8 TCDD	PCDD	HCDD	HPCDD	OCDD	TCDF	PCDF	HCDF	HPCDF	OCDF
		12-18	0									
62	1290N-410E	0-6	3.6									
63	1565N-150R	0-6	0									
		12-18	0									
	(Pile)	24-30	0.34									
		36-42	0.50									
		48-54	0.69	1.5	1.0	ND	ND	1.0	0.23	0.13	ND	ND

1	TCDD	=	tetrachlorodibenzodioxin
	PCDD	=	pentachlorodibenzodioxin
	HCDD	=	hexachlorodibenzodioxin
	HPCDD	=	heptachlorodibenzodioxin
	OCDD	=	octachlorodibenzodioxin
	TCDF	=	tetrachlorodibenzofuran
	PCDF	3	pentachlorodibenzofuran
	HCDF	3	hexachlorodibenzofuran
	HPCDF	3	heptachlorodibenzofuran
	OCDF	3	octachlorodibenzofuran

² ND means none detected.

II. Calculation of Equivalent Toxicity as 2,3,7,8-TCDD of CDDs and CDFs.

Procedures for determining the equivalent toxicity of a complex mixture of CDDs and CDFs are fully described in the Chlorinated Dioxins work group position document entitled "Risk Assessment Procedures for Mixtures of Chlorinated Dioxins and Dibenzo Furans (CCDs and CDFs)".

A copy of the document is attached as Appendix A. A summary of the procedure used to determine the equivalent toxicity of soil containing a mixture CCDs and CDFs follows; a sample calculation is included.

An estimate of toxic risks can be made by evaluating the CDD/CDF congeners or homologues which are estimated to have the greatest toxic potential. Toxicity data on many CDDs/CDFs are limited due to the lack of long-term studies. An interim approach for evaluating the toxicity of complex mixtures using "Toxicity Equivalent Factors" (TEF) has been recommended for determining risk. In utilizing this approach, components of CDDs and CDFs are identified and quantified. Based on structure-activity relationships, and the results of short-term tests,

the Chlorinated Dioxin work group assigned a relative toxicity factor to CDD/CDF isomers of most toxic concern (Table II). The product of the CDD/CDF concentration and the Toxicity Equivalent Factor converts the risk of a component of the mixture to the relative risk if that component were present as 2,3,7,8-TCDD. The equivalent risk of each component is added to obtain the total risk of the complex mixture as 2,3,7,8-TCDD.

TABLE II

CDD/CDF ISOMERS OF MOST TOXIC CONCERN 3/

Dioxin		Dibenzofuran						
<u>Isomer</u>	TRF b/	<u>Isomer</u>	<u> </u>					
2, 3, 7, 8-TCDD	1	2, 3, 7, 8-TCDF	0.1					
., 2, 3, 7, 8-PeCDD	0.2	1, 2, 3, 7, 8-PeCDF 2, 3, 4, 7, 8-PeCDF	0.1 0.1					
, 2, 3, 6, 7, 8-HxCDD	0.04	1, 2, 3, 6, 7, 8-HxCDF	0.01					
1, 2, 3, 7, 8, 9-HxCDD 1, 2, 3, 4, 7, 8-HxCDD	0.04 0.04	1, 2, 3, 7, 8, 9-HxCDF 1, 3, 4, 6, 7, 8-HxCDF	0.01 0.01					
L, 2, 3, 4, 6, 7, 8-HpCDD	0.001	1, 2, 3, 4, 6, 7, 8-HpCDF 1, 2, 3, 4, 7, 8, 9-HpCDF	0.001 0.001					

In each homologous group the relative toxicity factor for the isomers not listed above is 1/100 of the value listed above.

 $[\]underline{b}$ / TEF = toxic equivalency factor = relative toxicity assigned.

An example of the the calculation is presented in Table III. Sample Number 55 from a depth of 24"-30" at 980N, 430E was chosen because the tetra-, penta-, hexa-, hepta- and octachlorinated dioxins and dibenzofurans are present. The conservative assumption was made that all isomers of a specific polychlorinated group were present as the most toxic species of the group. For example, all pentachlorinated dioxin is assumed to be present in the mixture as 1,2,3,7,8 pentachlorodibenzodioxin.

TABLE III

Equivalent 2,3,7,8-TCDD Concentration of a Complex Mixture of CCDs/CDFs in Soil at Ethyl Petroleum Additives Plant Sauget, Illinois

Example of Calculation

Sample No. 55 Location:	980N, 430E	24"-	30" Depth
			Equivalent
	Concentration		Concentration
Constituent	<u>(ppb)</u>	<u>Tef</u> *	as 2,3,7,8, TCDD (ppb)
2.3.7.8-TCDD	39	1	39
PCDD	1.3	0.2	0.26
Hex CDD	4.5	0.04	0.18
Hep CDD	6. 6	0.001	0.007
Oct CDD	2.0	0	0
TCDF	26.2	0.1	2.62
PCDF	22.3	0.1	2.23 ·
Hex CDF	3.1	0.01	0.03
Hep CDF	0.98	0.001	0.001
Oct CDF	0.11	0	_ 0
		T	otal 44.328

^{*} TEF = Toxicity Equivalent Factor.

The results of the calculations for all data are presented in Table IV.

TABLE IV

Equivalent 2.3.7.8-TCDD Concentration of Soil Samples at Ethyl Petroleum Additives Plant Sauget, Illinois

Sample No.	Location	<u>Depth</u>	Total Equivalent 2,3,7,8-TCDD (All Species)
9	970N, 530E	12"-18"	0.319
10	930N, 560E	12"-18"	1.69
11	930N, 530E	12"-18"	161.427
12	880N, 530E	24"-30"	3.135
18	960N, 370E	24"-80"	109.024
24	980N, 430E	24"-30"	3.640
55	980N. 430E	24"-30"	44.328
57	930N, 430E	0 - 6"	7.773
63	1505N, 150E	48"-54"	1.200

Most of the samples were not from the surface of the ground. In order to estimate the equivalent concentration of 2,3,7,8-TCDD at surface levels, it was assumed that the chlorinated species would be present in the same relative concentrations throughout a core sample. The concentration of 2,3,7,8-TCDD was know at each location in the individual core. A ratio of the 2,3,7,8-TCDD at the surface to the 2,3,7,8-TCDD at any location in the core where the concentration of homologues and isomers of CDDs/CDFs had been determined would provide a factor to determine a reasonable estimate of 2,3,7,8-TCDD equivalent concentration at another location.

This ratio was calculated and equivalent 2.3.7.8-TCDD calculated at the surface. These data are preferred because the primary exposure route is believed to be due to inhalation of dust particulate. The data are summarized in Table V. An example calculation for Sample 55 follows.

Ratio = $\frac{2.3.7.8-\text{TCDD (Surface)}}{2.3.7.8-\text{TCDD (24"-30")}} = \frac{2.4 \text{ ppb}}{44.328 \text{ ppb}} = .0615$

Ratio x (Total Equivalent 2.3.7.8-TCDD 24"-30") = Total Equivalent 2.3.7.8-TCDD at Surface

(.0615)(44.328) = 2.73 ppb

TABLE V Calculated Equivalent 2,3,7,8-TCDD Concentration Soil at Bthyl Petroleum Additives - Sauget, Illinois

Sample No.	Location	Depth Inches	2,3,7,8-TCDD Isomer ppb	Total Equivalent 2,3,7,8-TCDD All Isomers Ppb	2,3,7,8-TCDD Isomer at Surface ppb	Modal	Equivalent 2,3,7,8-TCDD All Isomers at Surface
9	970N, 530B	12"-18"	0.31	0.319		Multiplier 1	ppb
10	930N, 560E	12"-18"	1.4		9.4	30.3	9.7
11	930N, 530E		1.6	1.69	2.6	1.625	4.0
		12"-18"	161.	161.427	51.		4.2
12	880N, 530E	24"-30"	3.0	2 125	31.	. 317	51.1
18	960N, 370E	24"-30"		3.135	110	36.67	114.9
24			107	109.024	100.	. 93	
	910N, 470E	12"-18"	3.2	3.640	2.4	.,,	101.9
55	980N, 430E	24"-30"	39		2.4	. 75	2.73
57	930N, 430E	0 - 6"		44.328	2.4	.0615	2.73
53			6.2	7.73	6.2	1.0	
J.	1505N, 150E	48"-54"	0.69	1.20		1.0	7.73
	is calculation				0	Not Applicable2	

¹ This calculation is not applicable for this core. The sample location is in a pile of dirt removed from a construction project on plant and has been disturbed and relocated.

² Multiplier = 2.3.7.8-TCDD at Surface 2.3.7.8 TCDD at Sample